

## **Speciation of Phosphorus and Sulfur in Mineral and Natural Systems**

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Beamline(s): **X19A**

**Introduction:** The use of synchrotron radiation in the 2000-3000 eV range at Beamline X19A of NSLS-BNL to study phosphorus and sulfur provides extremely valuable insight into the environmental chemistry of these elements in soils. Our research has found that it is possible to distinguish among calcium, ferrous, ferric, and calcium phosphate minerals using only XANES spectroscopy. Furthermore, the XANES spectrum of phosphate in aqueous phase as well as the spectra of phosphate adsorbed on iron and aluminum oxides are all substantially different from those of the various phosphate minerals. Using this knowledge, we have utilized XANES spectroscopy to speciate phosphorus in alum-amended poultry litter samples from southern Delaware. It was determined that alum amendments result in the formation of some sort of aluminum oxide which then adsorbs phosphate.

Additionally, sulfur K edge XANES spectroscopy was employed to study the bonding environment of sulfate in schwertmannite, or iron (III) oxy-hydroxy-sulfate. It was learned that there are pre-edge features diagnostic for sulfate bonding in the solid state with iron (III). Furthermore, there are distinct pre-edge features for monodentate sulfate as well as bidentate sulfate. Sulfate adsorbed as an inner-sphere or an outer-sphere surface complex lacks these features, and the spectra of adsorbed sulfate and aqueous sulfate are all identical. In the case of schwertmannite, the spectrum is also identical to that of aqueous/adsorbed sulfate, suggesting that there is no structural sulfate bound chemically in this mineral and instead it occurs as a counter-ion in the tunnel structure of this mineral. Previous studies that observed bidentate binuclear bonding of sulfate in schwertmannite likely are a result of sulfate adsorbed to schwertmannite as an inner-sphere surface complex.